

Report on Workshop II in SINE2020 WP 10 on Data Treatment



Group picture with the participants at Workshop II in WP10.

Venue:

Institut Laue-Langevin, Grenoble, France

Date

April 24 12:00 to April 25 15:00

Purpose

Presentation of guidelines and standards and how they should be used to exploit and interface to the software developed in this WP.

Presentation of considered software to early adopters and potential contributors.

Participants

There were 61 participants. Most of the participants belonged to one of the WP facility members, but there were also instrument scientists, users and developers from Oak Ridge National Laboratory in the US, Saint Petersburg Nuclear Physics Institute, the ESRF and the European Molecular Biology Laboratory.



Executive summary

In this document, you will find a summary of the second workshop, Workshop II, of WP10 in SINE2020, which took place at ILL April 24-25, 2017. The focus of the workshop was the first deliverable on Standard & Guidelines. Despite this rather technical topic, the number of participants exceeded the anticipations with 61 participants and with many external and potentials users (as opposed to developers from the member institutions of WP10). There were particularly many scientists from ILL and a few from neighboring institutions ESRF and EMBL, which was a desired outcome from letting ILL hosting the workshop.

The development of Standard & Guidelines for development of data treatment software was led by Anders Markvardsen from ISIS and was presented and discussed at the workshop in plenum. The discussion led to some modifications of the drafted guidelines. Besides this an overview of status and progress from the individual partners were also given in plenum.

There were parallel sessions scheduled for imaging, SANS, reflectometry, Mantid for continuous sources + QENS, and simulations. However, to promote synergies merged sessions between SANS and reflectometry and between Mantid, QENS, and simulations were scheduled. A simplified high-level programme is sketched below.

	Imaging (Anders K)	SANS (Wojciech)	Reflect. (Joachim)	Mantid + QENS (Ian + Miguel)	μ + Sim (Miguel + Thomas)
Monday	Plenum: Welcome and Standard & Guidelines				
	Dinner				
Tuesday					
		Joint session		Joint session	
	Plenum: Feedback + Conclusion				

A small group spun off from the simulation session in order to have a focused discussion and planning session for muon spectroscopy.

The data treatment software considered in this work package faces different challenges. The parallel sessions had accordingly different aims. More detailed descriptions for each of the parallel sessions are given later on, but some of the highlights were:

Imaging. It was announced that PSI has given the formal approval for converting MuhRec and KipTool to open source software, which is urgently needed for fostering joint collaboration on the same code base. Moreover it was decided to more strongly marketing the software at e.g. neutron imaging schools. Besides, an overview of different software programs used in neutron imaging was presented but also obtained from the participants.

SANS. This session had only few participants, most likely because it followed closely after a SasView codecamp. The participants represented however users from institutions that are not neutron sources, so the session was used to obtain user feedback. Moreover, a collaboration started with ESRF on usage of the ESRF SILX module (Scientific Library for eXperimentalists).

Reflectometry. Reflectometry is characterized by having many fragmented software programs available. The session was accordingly used to obtain input from users and developers of the most predominantly used software programs into a discussion on how a proper reflectometry analysis software program should look like.

Mantid for data reduction at continuous sources + QENS

In practice this was split into a session for Mantid on the first day, which focused on status updates and knowledge sharing between the continuum sources (ILL, MLZ/FZJ, and PSI) that are in the process of rolling out Mantid for data reduction at their instruments. Fitting software for QENS was the topic for the morning session on day two even though resources in WP10 has not yet been dedicated to this. The session high-lighted the lack of a widely accepted analysis software for QENS. In this regard, the situation for QENS mimics that of reflectometry. It was decided to organize a follow-up workshop specifically for QENS.

Muon spectroscopy, phonons and simulations

This session high-lighted that many facilities have development activities in this domain that are not well coordinated, and the need for more European coordination was emphasized. A spin-off group formed and successfully planned the next activities for the effort in WP10 on muon spectroscopy.

Standard and guidelines

A report on Standard and Guidelines for development of data treatment software for neutron scattering encompassed the first deliverable in WP10. The work on defining Standard and Guidelines was led by Dr. Anders Markvardsen from ISIS, who prior to writing the report had asked WP10 participants to complete a questionnaire for the software considered in this work package. Moreover, the developers of the McStas software, which is commonly used in the neutron scattering community, also completed the questionnaire.

The result of that questionnaire was discussed in plenum at the workshop, which resulted in comments and corrections that were included in the final report.

Parallel sessions

Below follows a brief summary for each of the parallel sessions.

Imaging

This session was organized and chaired by Anders Kaestner from PSI, who is the main responsible for the task on imaging in the WP. On the first day the session followed the program below;

16:30	Welcome (Anders Kaestner)
16:35	Status update (Anders Kaestner, Soren Schmidt)
16:50	How to promote a common tool suite?
17:10	Requirements (Anders Kaestner)
17:30	Reports from involved institutes
18:00	Computational imaging task force ISNR (Anders Kaestner)
18:30	Review open source visualization software (Chiara Carminati)

The imaging session was visited by developers from PSI, ESS, DTU, ISIS, and Oak Ridge (participation by means of web conferencing) and users from TU Delft, ILL, LLB, FZJ. The most important news was that the PSI codes MuhRec and KipTool are cleared to be released as open source. The preparations for the release are in progress and will happen during second half of 2017, the current focus is to release the next version of MuhRec. Partners are urgently waiting for the open source release of the code as it is considered to be essential for future collaboration on the same code base. The involvement of the International Society for Neutron Radiology (ISNR, www.isnr.de) was briefly mentioned, there is a task force to promote computational methods for neutron imaging. Reports about activities will be provided in the ISNR news letters

The webpage www.imagingscience.ch has had a workover changing the appearance, and added the ability to count downloads and offer newsletters. The visibility of the webpage must be improved to make it easier for search engines to find it.

During the round table status report by the participants each reported their suite of tools for neutron imaging data reduction and analysis. Octopus (commercial), MuhRec, TomoPY, and ASTRA toolbox were mentioned for computed tomography. Typical analysis tools used among the participants were scripting based using either Matlab or Python and GUI based 3D rendering software like VGStudio (commercial) or open source tools like Drishti or 3D slicer. Dr. Chiara Carminati presented an overview of open source visualization software among others Drishti, 3DSlicer, and TomViz. The latter two are both based on KitWare libraries. There was general interest in python based solutions, many have left or are considering leaving Matlab in favor of python as analysis tool. This puts emphasis on the importance to interface developed algorithms to python.

Information about the existence of the tool suite developed at PSI has until now mainly been distributed to the PSI user community. To change this, it was concluded that the tools should be promoted during imaging schools. The tools shall also be more widely presented at conferences and workshops to increase the visibility. Also, there will be a newsletter to inform current users about new releases etc.

On the second day, the time was devoted to hands-on sessions for people interested in learning to use MuhRec and / or KipTool. The typical reconstruction workflow was demonstrated; first as a basic reconstruction, then adding more advanced artifact cleaning techniques to remove lines and rings in the reconstructed data. Many neutron imaging experiments are performed on the limits of the instrument performance and in particular the neutron doses used are relatively low with low signal to noise ratio as consequence. A denoising filter in KipTool was demonstrated and the SNR was increased radically. The code design of the module system and some code highlights relevant for the low-level integration of the components were presented after the software demonstration sessions. This part was appreciated by several of the participants.

SANS

This session on analysis software for SANS was organized and chaired by Dr. Wojciech Potrzebowski from ESS, who is one of the lead developers of SasView in this WP. The session took place over both days of the workshop with the following program:

16:30	Welcome (Wojciech Potrzebowski)
16:35	SasView v4 - Data analysis for small angle scattering (Andrew Jackson)
17:25	Online SAXS data reduction at the ESRF - the European Synchrotron (Jerome Kieffer)
17:50	Small Angle Scattering software love and hate. User experience at X-ray and neutron facilities (open discussion)

9:00	New SasView GUI (Piotr Rozycko)
9:45	SasView CLI and models library (Wojciech Potrzebowski)
10:30	Coffee break

11:00	SasView tutorial and documentation (Wojciech Potrzebowski and Piotr Rozycko)
11:30	Open discussion together with participants on session on reflectometry (at Chadwick Amphi)

The SasView parallel session gathered beam line scientists and software developers from the neutron sources ILL, ISIS, and ESS, but also from the European Synchrotron Radiation Facility

(ESRF), the European Molecular Biology Laboratory (EMBL) and University of Bath. All together the session was attended by seven persons. The participants of the session had experience with various software for analysis of small angle scattering data with none to extensive prior experience with SasView. The participants covered a wide range of domains and thus had different requirements to SasView.

The main goal of the session was to discuss the recent developments for SasView in the framework of SINE2020, which involve modularization, user interfaces and the extension of the model library with SASFit models. The feedback from the presentation of the new GUI design was in general positive and the improvement over the previous version of SasView GUI was noted. The plans for the future developments were also well received including the plan to replace the current plotting module with silx (<https://github.com/silx-kit/silx>) developed at ESRF. One of the silx developers from ESRF participated in the session and thus provided immediate feedback on issues raised, e.g. on how to add context menus to silx charts. Several improvements to the SasCalc module in SasView were suggested by the participants, for instance on-the-fly compilation with numba (<http://numba.pydata.org/>) and potential simplification of model functions in order to solve scientific problems with less complicated and time-consuming model functions. To this end, the implementation of some of the already existing models may be revisited.

The current limitations of SasView and potential avenues for extensions were also addressed. In particular, tools for structural biology were discussed. These involved the addition of hydration layers to models, the calculation of the scattering intensity from single or multiple PDB files and consecutively calculating the agreement with experimental data (using χ^2 or other figure of merit), population weights inference from mixture of species and the inclusion of a bead (dummy) model generator. It was decided that the minimal requirement for SasView from the structural biology community is that it can calculate the scattering pattern from an atomic protein structure (e.g. in the PDB format) and that the generic scattering calculator should be extended so that it can handle different levels of deuteration. In addition to requirements for structural biology, the options to use different figures of merit and simultaneously fit SAXS and SANS data were also requested and treatment of 2D data was discussed. These requirements and discussions will now be considered in the future plans for development of SasView in SINE2020.

In addition to the discussions specifically on SasView, there was also a discussion dedicated to the user experience related to the use of data analysis software for small angle scattering data. A questionnaire to facilitate discussion was sent out prior to the meeting. Based on the answers in the questionnaire, a number of good and bad software development practices were discussed. It was emphasized that the efforts in WP10 for providing reliable, sustainable, maintainable and inter-operable software are very much in line with good software development practices and should diminish negative user experiences in the future.

Reflectometry

The session for reflectometry was organized and chaired by Dr. Joachim Wuttke, who is head of the scientific computing group at FZJ/MLZ and one of the lead developers of BornAgain. The sessions took place over both days of the workshop with the detailed program below;

16:30	Welcome (Joachim Wuttke)
16:35	Standard and off-standard uses of ILL reflectometers; standard data analyses (Philipp Gutfreund)
16:55	10 years with GenX - past present and future (Matts Björck)
17:25	Reflectometry Data Analysis Software – ISIS Requirements and Strategy (Arwel Hughes)
17:50	From simple layer models over complex magnetic superstructures to single pulse reflectivities at ESS - Reflectivity analysis from an instrument scientists perspective (Artur Glavic)
18:20	[cancelled due to illness of the speaker; time was used up by longer discussions of other talks]
18:35	Needs of users in the area of soft and biological thin films (Yuri Gerelli)
18:45	Data analysis needs for soft matter and biology (Hanna Wacklin)

10:00	Coherent and incoherent averaging in evaluation of Off-specular scattering and GISANS (Boris Toperverg)
10:30	Coffee break
11:00	Modelling and fitting GISAS with BornAgain - status and plans (Walter Van Herck)
11:30	Open discussion together with participants on session on SasView

In this session, the status and future of reflectometry software were discussed from two main viewpoints. Developers and maintainers of reflectometry software packages demonstrated the functionality of the software and their future plans with it. Instrument scientists and experienced reflectometer users showed their current workflow and expressed requirements for reflectometry software.

After an introductory welcome, Philipp Gutfreund gave an overview of the data analysis workflow at ILL reflectometers. He provided a list of relevant software packages, and indicated their strengths and limitations.

Matts Björck gave an overview of GenX functionality accumulated during 10 years of development and reported recent improvements done in the GenX package. He concluded by showing interesting results of using GenX in client/server mode.

Arwel Hughes reported his recent progress and development plans related to the Matlab based application Rascal 2, a data analysis software at ISIS.

Artur Glavic gave us his personal list of reflectometry software requirements, which included a part for newcomers and another one concerning scientists with advanced software background. He also showed a few interesting and challenging experimental geometries which are under investigation at PSI at the moment.

Yuri Gerelli explained us his needs for biologically relevant thin film geometries and especially pointed out the necessity of a linked fit parameter mechanism. Finally, he stressed the importance of a correct error calculation for highly correlated fit parameters.

Hanna Wacklin presented the data analysis needs in the fields of soft matter and biology, and gave a concise MotoFit tutorial.

The author of MotoFit, Andrew Nelson, could not come over from Australia, but he sent a detailed message to the workshop attendees. As MotoFit depends on the proprietary platform IgorPro, he is currently experimenting with a Python package refnx.

Boris Toperverg shared valuable insights from his longstanding experience with magnetic GISANS analysis.

Walter Van Herck started with an overview of the status and future plans of the BornAgain software package. The second part was devoted to a demonstration of the current functionality of the software package.

Mantid for data reduction at continuous sources

The session for Mantid took place on the first day of the workshop with the following program;

16:30	Welcome (Ian Bush)
16:35	Mantid at MLZ: status and future plans (Marina Ganeva)
16:55	Mantid at PSI: status and future plans (Emmanoela Rantsiou)
17:15	Mantid at ILL (Verena Reimund, Gagik Vardanyan, Antti Soininen, Ian Bush)
18:00	Discussion

The session was organized jointly by Ian Bush, ILL and Tesella, and Miguel Gonzalez, ILL, and chaired by Ian Bush. They are both lead developers of Mantid for data reduction at ILL.

The primary goal of the session was to share experiences and knowledge regarding the implementation of Mantid for data reduction at the continuous sources ILL, SINQ (PSI), and FRM-II (FZJ/MLZ).

The session started with an introduction from all of the participants to where they are from and what their background is.

Marina Ganeva from the MLZ then started with a summary of the status and future plans for work in Mantid at the MLZ. TOFTOF is in production, and being maintained. DNS in diffraction mode is in commissioning, expected to be used in May 2017. DNS TOF/TOPAS is in development, as is POWTEX. SPHERES and SANS-1 have been requested.

Marina gave an overview of training sessions ran at the MLZ, including some feedback from the users. The users all broadly found it useful, although had different prior skills and expectations

from the workshop. They found from this that some users need a simple GUI, some need simple linear Python scripts and the overall data reduction must be flexible.

Marina then showed an overview of the data reduction for TOFTOF, DNS and POWTEX. There were a number of issues that may need addressing in Mantid, such as support for ragged workspace, unit conversion in 2D data sets, normalization to bin area and 2D fitting.

Emmanouela Rantsiou from the PSI gave an update on their Mantid work for SINQ. The long term plan is to make Mantid the standard data reduction tool, with development of custom made algorithms for all SINQ beamlines. Currently some work has been done to read the standard SINQ Nexus and HDF files. Some beamline specific Mantid algorithms are also included currently in the Mantid distribution.

Work has been done for the AMOR reflectometer, to port existing data reduction and analysis workflow scripts into Mantid. The first version is completed, and it is expected to be included in the upcoming SINQ cycle. There have also been developments to support some of the operation modes on the BOA beamline.

Emmanouela mentioned some issues with Mantid on SL6. They are now transitioning to RHEL7 which works much more easily. The talk was followed by some discussion on how best to document workflows, whether these should be aimed at users or instrument scientists. There was also some discussion of how to write documentation for Mantid specifically.

Finally Verena Reimund, Gagik Vardanyan, Antti Soininen and Ian Bush gave an update on the work at the ILL. They started off with a brief overview, work is well advanced for Time-of-Flight spectroscopy and Backscattering. Work has now started on Reflectometry and Powder Diffraction, as well as framework changes to support scanning instruments at the ILL. Future work is planned for SANS and other technique areas.

The workflow and details of the implementation for Backscattering were explained for QENS and FWS reductions. A comparison against the existing LAMP software was also shown. For Time-of-Flight reduction a similar explanation was given for the workflow, which has been divided into chunks for easier use. A comparison against LAMP was also made, and the reasoning behind some of the differences between LAMP and Mantid after $S(Q, \omega)$ conversion.

Finally they talked about the scanning instrument (instruments with moving detector work) that the ILL and the ESS have been involved in. They explained some of the technical details and motivation behind this, and showed a view on a loaded D2B workspace.

After the talks some further discussion was related to the approach to workflows, which has been similar, but slightly different at the three institutes. The approach here can largely depend on the requests of the instrument scientists, and the complexity of the data reduction.

Marina Ganeva was interested in the work on the scanning instruments, which should be applicable to the DNS instrument. There was interest in access via Python functionality, though this is not available yet. Ian and Marina will continue to talk about this after the workshop.

Simulations

The detailed program for the sessions on simulations on the first day of the workshop is shown below;

16:30	Welcome (Roberto De Renzi, Stephen Cottrell, Thomas Holm-Rod)
16:35	Status, plan and messages from muon group (Roberto De Renzi, Stephen Cottrell)
16:50	Status, plan and messages from ILL (Miguel A. Gonzalez)
17:05	Status, plan and messages from ESS (Thomas Holm Rod)
17:20	Introduction to the MAX European Centre of Excellence (Pietro Bonfa)
17:40	Status, plan and messages from SNS (Jose Borreguero)
17:55	Status, plan and messages from ISIS (Anders Markvardsen)
18:10	Discussion, working groups, demo, hands-on ...

The session consisted mainly on presentations from the partner facilities (ILL, ESS, ISIS) on their current efforts, plans and interests concerning the use of simulations to enhance the output of the neutron experiments performed at them. Jose Borreguero (ORNL) also presented the independent efforts that are being pursued at SNS in the same direction and Pietro Bonfà (Cineca) introduced the MaX Center of Excellence for HPC applications.

From the ILL side, Miguel A. González talked about the past activities of the Computing for Science group aiming to develop the combined use of simulations and neutron data. The most visible output of this effort is MDANSE, developed by Eric Pellegrini (ILL) and based on two previous collaborations between ILL and the University of Orleans and financed by the French ANR. This code is freely available and allows to analyse Molecular Dynamics trajectories and compute neutron observables. At present, the institute prioritizes the development of adequate tools to compute inelastic neutron scattering data. In particular, a software solution to calculate the vibrational densities of states measured in the Lagrange spectrometer is urgently needed. For this, collaboration with the ISIS scientists developing AbINS in Mantid is envisaged. Additional tools to compute phonon dispersion curves and the inelastic dynamic structure factors (both for single-crystal and powders) typically measured in the triple-axis and TOF spectrometers are also needed.

Thomas Holm Rod presented the situation at ESS. Efforts on modelling are still modest, but will be increased once the construction phase is finished and a fully independent group on Computational modelling, simulation and theory is created. In the meantime, several isolated projects funded by external partners (mainly the Swedish Research Council and Swedish Universities) have been started and involve already ESS staff, possibly becoming the embryo of the future modelling activities at ESS.

The situation at ISIS was presented by Sanghamitra Mukhopadhyay. In recent years ISIS has done a great effort to develop computational tools facilitating the link between simulation and experiment, mainly using the framework provided by Mantid. One of those efforts is AbINS,

implemented as a plugin to Mantid to calculate INS spectra from ab-initio lattice dynamics. Future developments in AbINS will include also the calculation of 2D (Q, ω) maps. Other smaller developments done at ISIS involve the creation of Mantid interfaces to read and manipulate output files from nMoldyn (the ancestor of MDANSE), thus facilitating the comparison of simulation and experiment.

In parallel with the efforts foreseen in the European project, similar work is being done in an independent way at ORNL, as shown by Jose Borreguero. He presented ACUMEN, a project aiming to develop scalable mathematical research useful for neutron science, and BEAM, a computational workflow system to facilitate the access of instrument scientists to HPC resources. Those tools are already being used to compute phonon-dispersion relations from DFT calculations and refine force constants, as well as to perform virtual experiments in spectroscopy (analogous to the goal pursued with AbINS). The discussion that followed this presentation showed the common interests shared by neutron facilities and it was agreed that the contacts and possibly the collaboration between the European partners in SINE2020 and ORNL should increase.

Finally Pietro Bonfà (Cineca, Italy) introduced the MaX European project, which is aiming to enable the exascale transition (10^{18} floating-point operations/s) by developing novel algorithms and programming models. He showed that in the near future neutron scattering users could benefit from the simulation codes (many already in use and well known by the community) and the workflows set in place in the framework of this initiative.

Muon spectroscopy

After the simulation session on the first day, a breakout group of four persons formed that focused entirely on analysis software for muon spectroscopy with a focus on technical aspects of the project.

They took a forward look to the code release, making a decision about how the C++ library is to be handled (compiled for three platforms), agreeing a subset of existing routines to document for release, and agreeing a timescale of a few months for Pietro to finalize the code for release.

They also discussed options for hosting the software, that this is likely to start off with the routines being available for download from the Mantid Script Repository although placing the code as 3rd party software may be considered in the future.

An agreement was made to develop three case studies (LiFePO₄, Fe(bcc) and MnSi) to present on release, and agreed that these should be in the form of mini-lectures to make the scientific motivation, the case for a muon study, the advantage that the software package gives and the results from the study clear and understandable to a young scientist/non-specialist. It will be considered to use the case studies, etc, for presentations at future muon schools, site calculation workshops and other suitable meetings. Moreover, it was agreed to develop a tutorial to help people getting started with the software.

Finally, methods for communication/dissemination of the software and scientific possibilities were discussed. The need to place this work in the context of other efforts in this area (grant to Oxford/Durham/RAL and project with SCD) was recognised. The muonsources.org website will be used as a centre point for collecting information about this work.

QENS

The QENS session took place in the morning on the second day of the workshop. The detailed program is below;

9:00	Experiences from Frida: the cryptic command line saga (Joachim Wuttke)
9:20	Recent developments on QENS analysis in Mantid (Sanghamitra Mukhopadhyay)
9:40	QENS at SNS (Jose Borreguero)
9:50	QENS at PSI: user's and instrument scientist's point of view (Fanni Juranyi)
10:10	QENS at ILL: Tools in Lamp (Miguel A. Gonzalez)
10:20	QENS at ESS (Celine Durniak)

Following on from the Mantid and simulation session on the first day of the workshop, the session devoted to the software for the analysis of QENS data, which took place on the second day, was attended by about 20 scientists and consisted on 6 presentations reflecting the present situation and expectations at different facilities.

Overall the presentations showed the large variety of needs that a QENS analysis package should fulfil and the absence of a single well accepted solution in the community. For example, Joachim Wuttke (MLZ) presented his own software Frida, which is extremely flexible and can be used both for data reduction and analysis. However the absence of a user interface and a user manual make it very hard to adopt for new users. On the other hand, Fanny Juranyi (PSI) presented DAVE (developed at NIST), which is very user friendly but lacks some flexibility to tie parameters and fit simultaneously more than one data set using some common fitting parameters. She also pointed to the need of having a very simple tool to perform quick fits during the data acquisition. Miguel A. González (ILL) talked about the situation at the ILL, where many different programs are used by scientists and users as no single one meets the requirements of all of them. Sanghamitra Mukhopadhyay (ISIS) presented the recent developments on QENS data analysis that the ISIS team is implementing in Mantid. They include a library of models and the possibility of using several minimizers, including a Bayesian one (Fabada). They make Mantid a promising framework that could provide a unique environment to perform both the data reduction and analysis for both QENS and INS experiments. The Mantid framework is also being used for this purpose at SNS, as José Borreguero (ORNL) explained. He presented the independent developments that ORNL is pursuing in the field of QENS fitting, as well as their efforts to combine experiment and simulation in the analysis workflow. Finally Céline Durniak (ESS) presented the perspective and preliminary requirements expected at ESS, where it is foreseen that at least 5 instruments would benefit from the developments discussed in the session.

During the discussion, many of the points raised during the presentations were considered, reaching some consensus on what users and scientists expect from software used to fit QENS data. Thus it should have a friendly user interface and a well-established library of models and methods in order to allow new or inexperienced users to be able to fit easily and quickly their data, minimizing also the possibility of misuse. But at the same time it should be fully scriptable and

flexible enough to allow expert users to add new models and constraints, as well as to setup more complex fitting workflows. It should allow the use of different fitting algorithms (e.g. Levenberg-Marquardt, Bayesian, Monte Carlo, Genetic Algorithms, etc.) and provide a complete analysis of the results, including reliable estimates for the uncertainties of the fitted parameters. Good documentation and tutorials should also be provided. Ideally it should allow to combine easily measurements performed in different instruments or even using different techniques. Other requests include the ability to save and load the complete fitting session, to run on multiple cores/GPUs and clusters and to produce publication-quality figures.

Another objective proposed was to provide an independent library of QENS models that could be used by different fitting programs. It was also recognized that the efforts already done in Mantid represent a good starting point in order to devise a complete tool for QENS analysis fulfilling most of the goals mentioned above. Future discussions will take place between scientists of the different facilities in order to make further progress in this sense.

Furthermore, it was decided to organize a follow-up workshop on QENS fitting to work on outstanding questions raised in this section and also as part of working towards the 42 months deliverable D10.6 QENS(Mantid) ready for user test.

Enclosure A: Programme

Programme

Monday 24th April 2017

- 12:00** Registration and lunch
- 13:30** Welcome (*Chadwick Amphi*) Thomas Holm Rod
- 13:40** Update on project status and news from partners Thomas Holm Rod + others
- 15:00** Guidelines and standards Anders Markvadsen
- 16:00** Group photo
- Coffee break
- 16:30** Parallel sessions

Mantid for continuous sources (*ILL4 S121*)

16:30	Welcome (Ian Bush)
16:35	Mantid at MLZ: status and future plans (Marina Ganeva)
16:55	Mantid at PSI: status and future plans (Emmanoela Rantsiou)
17:15	Mantid at ILL (Verena Reimund, Gagik Vardanyan, Antti Soininen, Ian Bush)
18:00	Discussion

Muons, simulations and phonons (*ILL4 Seminar Room*)

16:30	Welcome (Roberto De Renzi, Stephen Cottrell, Thomas Holm-Rod)
16:35	Status, plan and messages from muon group (Roberto De Renzi, Stephen Cottrell)
16:50	Status, plan and messages from ILL (Miguel A. Gonzalez)
17:05	Status, plan and messages from ESS (Thomas Holm-Rod)
17:20	Introduction to the MAX European Centre of Excellence (Pietro Bonfa)
17:40	Status, plan and messages from SNS (Jose Borreguero)
17:55	Status, plan and messages from ISIS (Anders Markvadsen)
18:10	Discussion, working groups, demo, hands-on ...

Reflectometry (*Chadwick Amphi*)

16:30	Welcome (Joachim Wuttke)
16:35	Standard and off-standard uses of ILL reflectometers; standard data analyses (Philipp Gutfreund)
16:55	10 years with GenX - past present and future (Matts Björck)
17:25	Reflectometry Data Analysis Software – ISIS Requirements and Strategy (Arwel Hughes)
17:50	From simple layer models over complex magnetic superstructures to single pulse reflectivities at ESS - Reflectivity analysis from an instrument scientists perspective (Artur Glavic)
18:20	Challenge to constrain parameters in multi-layer reflectometry modeling of surfactant systems to be physically realistic (Richard Campbell)
18:35	Needs of users in the area of soft and biological thin films (Yuri Gerelli)
18:45	Data analysis needs for soft matter and biology (Hanna Wacklin)

SasView (*ILL4 S158*)

16:30	Welcome (Wojciech Potrzebowski)
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16:35	SasView v4 - Data analysis for small angle scattering (Andre)
17:25	Online SAXS data reduction at the ESRF - the European Syn
17:50	Small Angle Scattering software love and hate. User experier facilities (open discussion)

Imaging (*ILL4 164, videoconference room*)

16:30	Welcome (Anders Kaestner)
16:35	Status update (Anders Kaestner, Soren Schmidt)
16:50	How to promote a common tool suite?
17:10	Requirements (Anders Kaestner)
17:30	Reports from involved institutes
18:00	Computational imaging task force ISNR (Anders Kaestner)
18:30	Review open source visualization software (Chiara Carminat)

19:00 Transport to town (Tramway B)

19:30 Dinner (Fantin Latour)

Tuesday 25th April 2017

9:00 Parallel sessions (cont)

QENS analysis (*ILL4 seminar room*)

9:00	Experiences from Frida: the cryptic command line saga (Joa)
9:20	Recent developments on QENS analysis in Mantid (Sanghan)
9:40	QENS at SNS (Jose Borreguero)
9:50	QENS at PSI: user's and instrument scientist's point of view
10:10	QENS at ILL: Tools in Lamp (Miguel A. Gonzalez)
10:20	QENS at ESS (Celine Durniak)

Muons, simulations and phonons (*ILL4 S121*)

9:00	Discussion, working groups, demo, hands-on ...
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Reflectometry (*Chadwick Amphi*)

10:00	Coherent and incoherent averaging in evaluation of Off-spec (Boris Toperverg)
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SasView (*ILL4 S158*)

9:00	New SasView GUI (Piotr Rozycko)
9:45	SasView CLI and models library (Wojciech Potrzebowski)

11:30	Open discussion together with participants on session on SasView
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SasView (*ILL4 S158*)

11:00	SasView tutorial and documentation (Wojciech Potrzebowski and Piotr Rozycko)
11:30	Open discussion together with participants on session on reflectometry (at Chadwick Amphi)

Imaging (*ILL4 164, videoconference room*)

11:00	Hands-on session
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12:30 Lunch

13:15 Feedback from parallel sessions

Discussion and coordination

Organization of next workshop

14:45 Closing remarks

15:00 Departure

Enclosure B: Participant list

No	Name	Institution	No	Name	Institution
1	ARAMINI, Matteo	STFC	31	JURANYI, Fanni	PSI
2	BILHEUX, Jean	ORNL, USA	32	KAESTNER, Anders	PSI
3	BJÖRCK, Matts	Scattered Sci, SE	33	KIEFFER, Jerome	ESRF, FR
4	BOEHM, Martin	ILL	34	LIM, Anthony	STFC
5	BONFÀ, Pietro	CINECA, IT	35	MARKVARDSEN, Anders	STFC
6	BORREGUERO CALVO, Jose	ORNL	36	MARTEL, Anne	ILL
7	BRENNICH, Martha	EMBL Gren., FR	37	MCCLUSKEY, Andrew	Univ. Bath, UK
8	BURLE, Jan	FZJ	38	MUKHOPADHAY, Sanghamitra	STFC
9	BUSH, Ian	ILL / Tessella	39	MUTTI, Paolo	ILL
10	CAMPBELL, Richard	ILL	40	NIELSEN, Torben	ESS
11	CARMINATI, Chiara	PSI	41	OLLIVIER, Jacques	ILL
12	COTTRELL, Stephen	STFC	42	PIAZZA, Irina	ILL
13	DALGLIESH, Robert	STFC	43	POSPELOV, Gennady	FZJ
14	DE RENZI, Roberto	UNIPR	44	POTRZEBOWSKI, Wojciech	ESS
15	DURNIAK, Celine	ESS	45	PREVOST, Sylvain	ILL
16	EXIL, Gaston	CEA/LLB	46	RANTSIOU, Emmanouela	PSI
17	FAK, Bjorn	ILL	47	REIMUND, Verena	ILL
18	FEDRIGO, Anna	ESS	48	ROD, Thomas	ESS
19	FISHER, Jonathan	FZJ	49	ROZYCZKO, Piotr	ESS
20	FOUQUET, Peter	ILL	50	SCHMALZL, Karin	FZJ
21	GANEVA, Marina	FZJ	51	SCHMIDT, Søren	DTU
22	GERELLI, Yuri	ILL	52	SOININEN, Antti	ILL
23	GLAVIC, Artur	PSI	53	TASEV, Dimitar	ISIS
24	GONZALEZ, Miguel Angel	ILL	54	TAYLOR, Jonathan	ESS
25	GUTFREUND, philipp	ILL	55	TENGATTINI, Alessandro	ILL
26	HAFNER, Aljosa	ILL	56	TOPERVERG, Boris	PNPI, RUS
27	HONECKER, Dirk	ILL	57	VAN HERCK, Walter	FZJ
28	HUGHES, Arwel	ISIS	58	VARDANYAN, Gagik	ILL
29	JACKSON, Andrew	ESS	59	WACKLIN, Hanna	ESS
30	JORGJI, Emiljana	LLB	60	WUTTKE, Joachim	FZJ
			61	ZHOU, Zhou	TUD

(Signed list is archived by the WP leader)

Enclosure C: Expenses

Participants paid for their own travel and accommodation. Usage of meeting rooms were provided for free by ILL. Thus, the only cost to the workshop was for two times lunch, dinner, and coffee, which added up to € 4111.20.

Libellé	Dépenses TTC
TICKETS TRANSPORTS TAG (3 X 30 TICKETS)	117,00 €
RESTO LE FANTIN LATOUR, 24/04/17, 54 couverts	2 700,00 €
CARTES CANTINE INVITES 04/17	708,10 €
SANDISK + LEXAR PRO SD HC	97,70 €
PAUSES CAFE	488,40 €
TOTAL	4 111,20 €
Meeting SINE2020, 24/25 Avril 2017	
Ligne budgétaire 96000V569706	